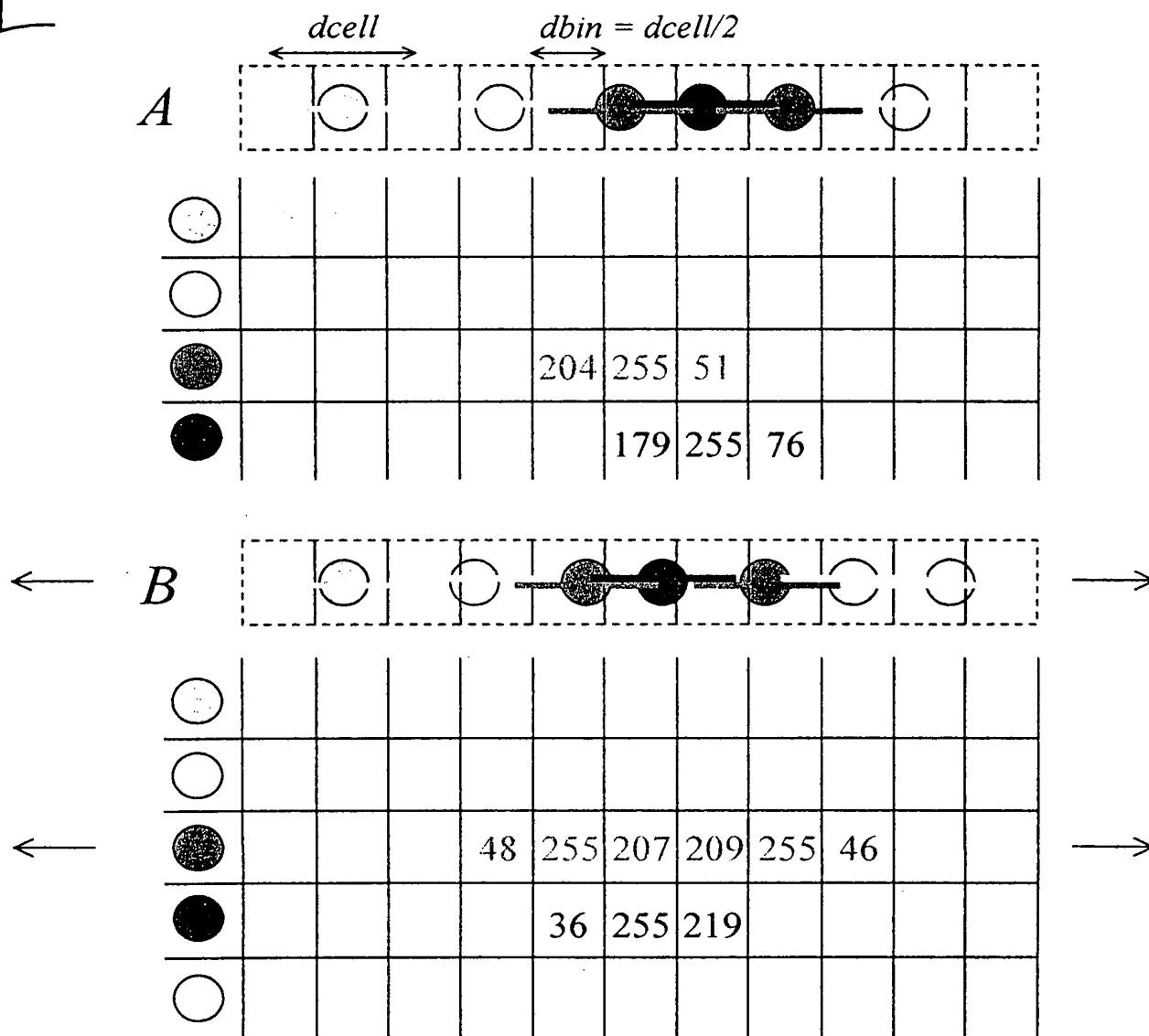


Bin-Based Overlap

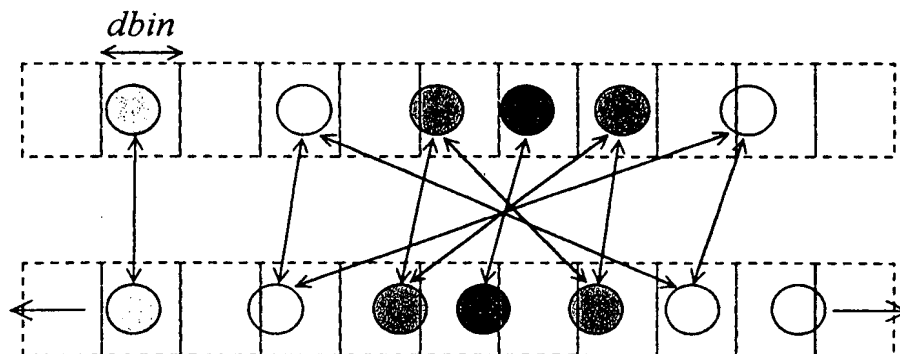
- Do a series of fast overlap calculations using “bins” with integer occupation numbers (0→255) for each atom:



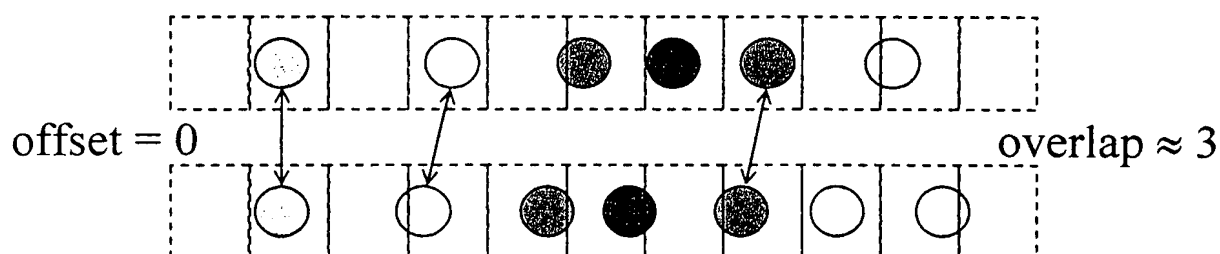
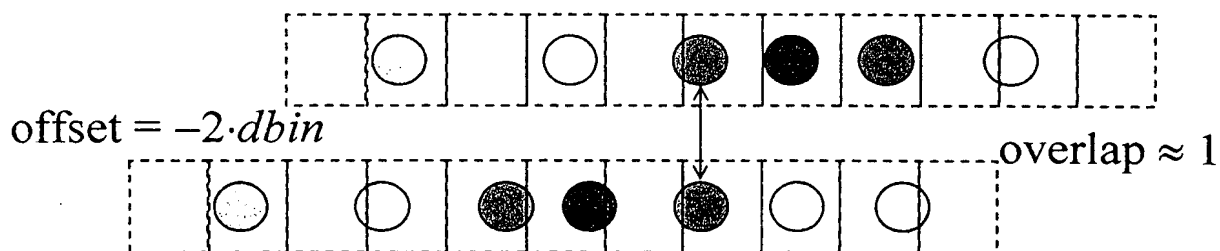
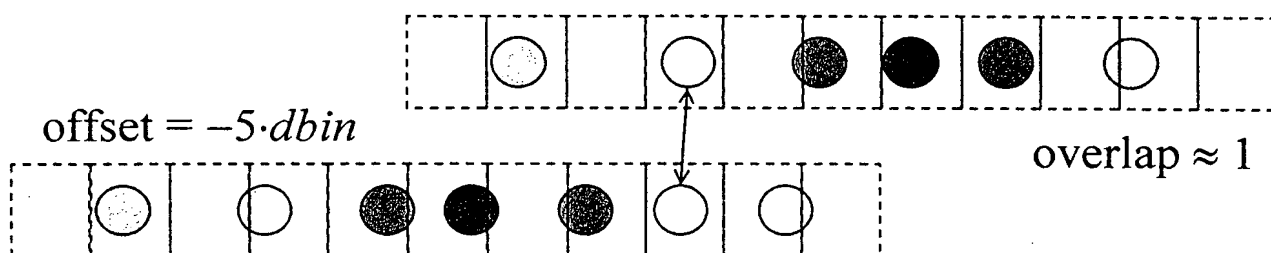
- Multiply occupation numbers for matching atom types across aligned bins to get a good estimate of overlap area
- Fast, but there are numerous bin-based offsets that must be considered

FIG. 13

Speeding Up Bin-Based Overlap Calculations



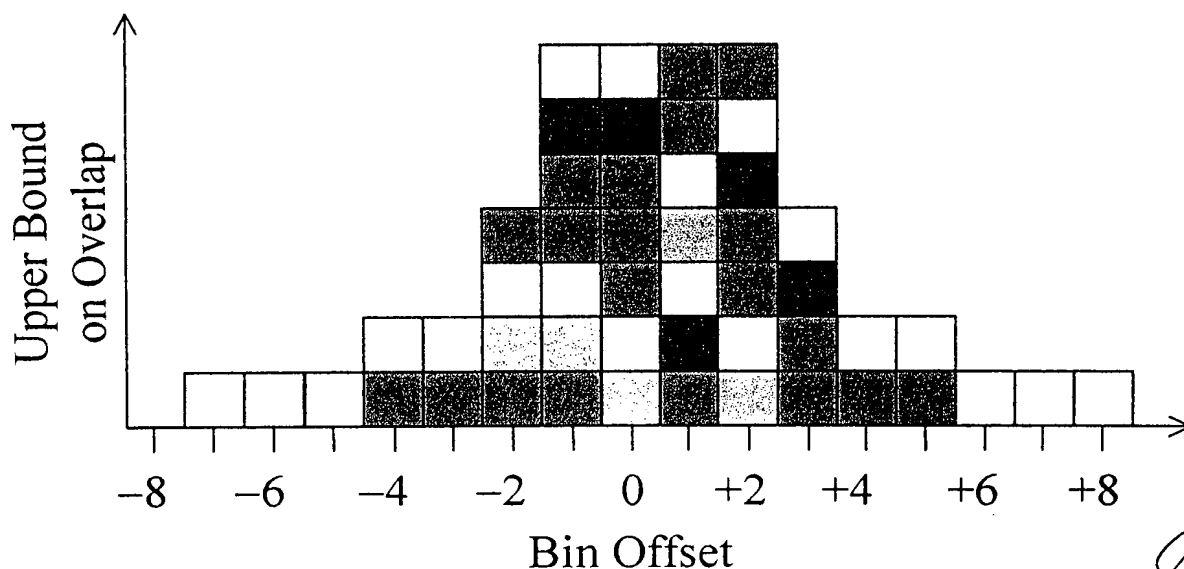
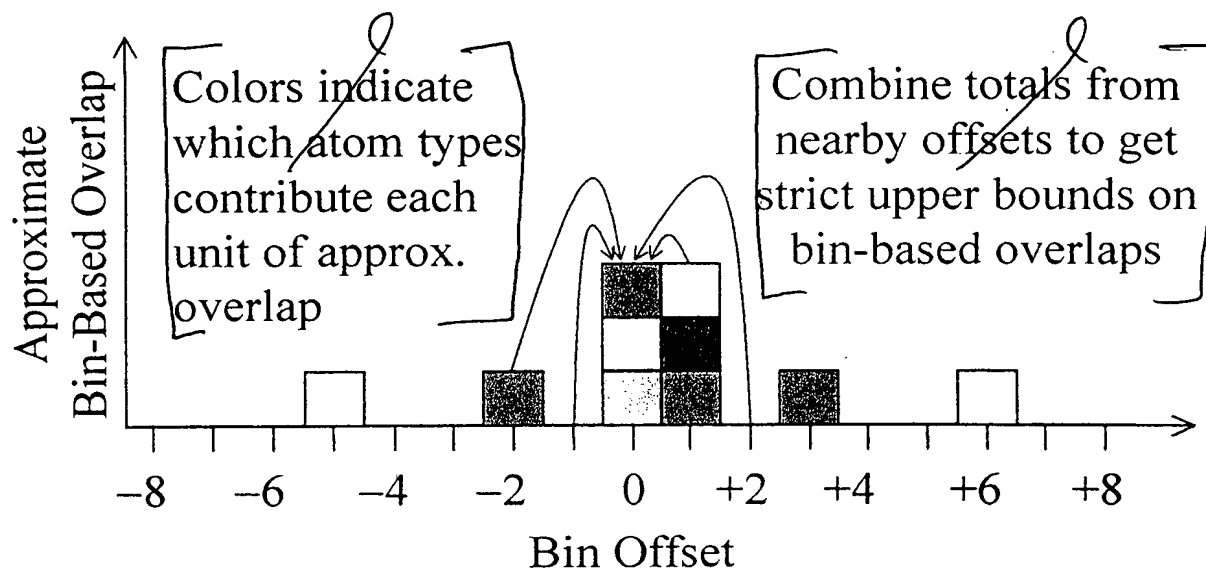
- 21 unique bin offsets, 10 matching atom type pairs
- There are only 6 different bin offsets wherein matching atom types are approximately aligned:



etc.

FIG. 14

Approximate Bin-Based Overlaps → Upper Bounds



- Process offsets in order of decreasing upper bound
- Do standard bin-based overlap calculations (with occupation numbers), keeping track of the largest overlap value
- Stop when remaining upper bounds are lower than this largest bin-based overlap

FIG. 15

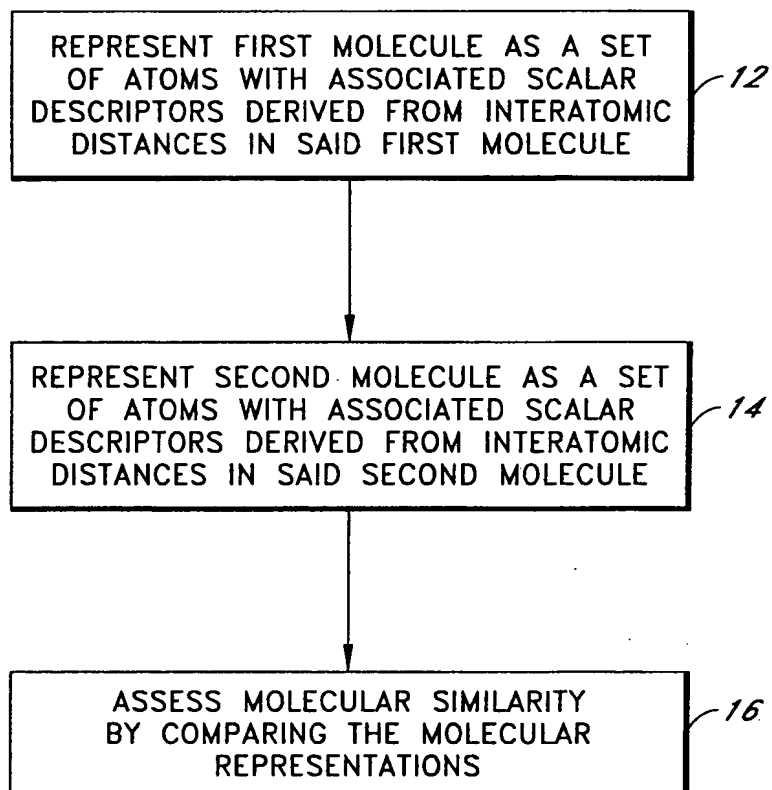


FIG. 1

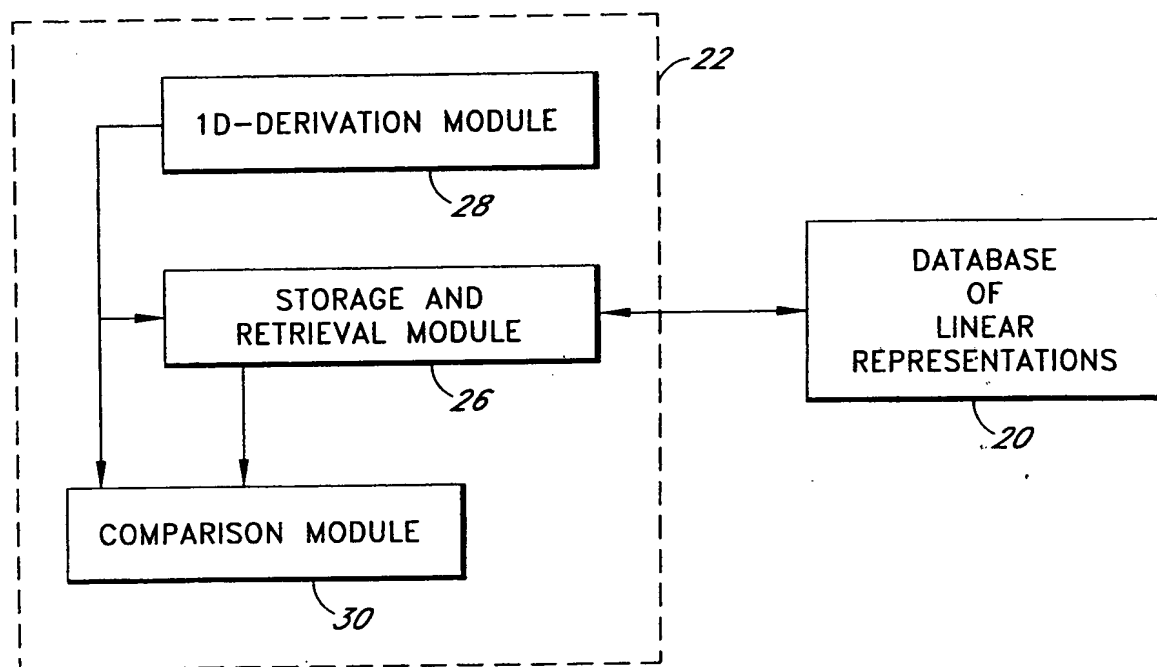


FIG. 2

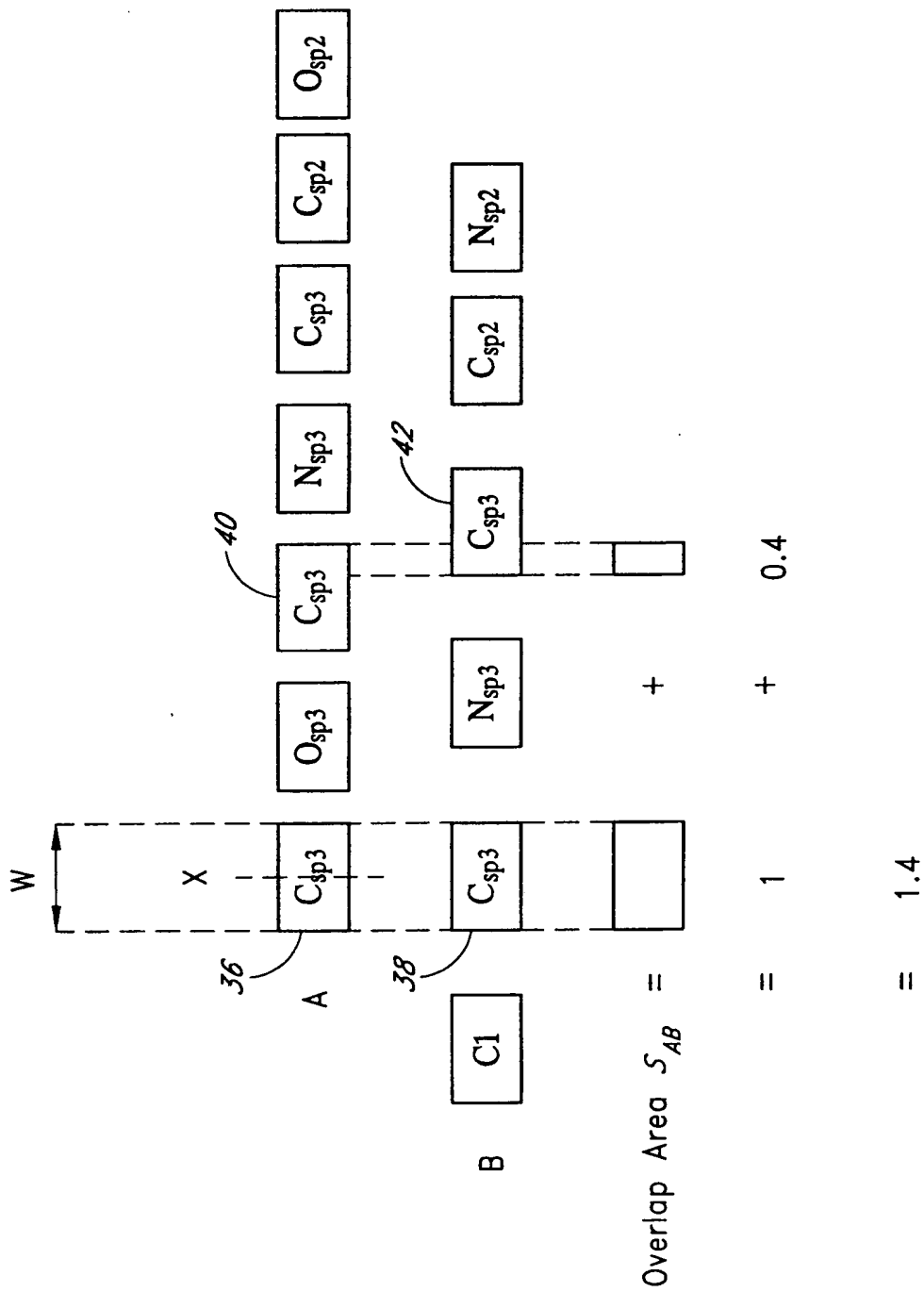


FIG. 3A

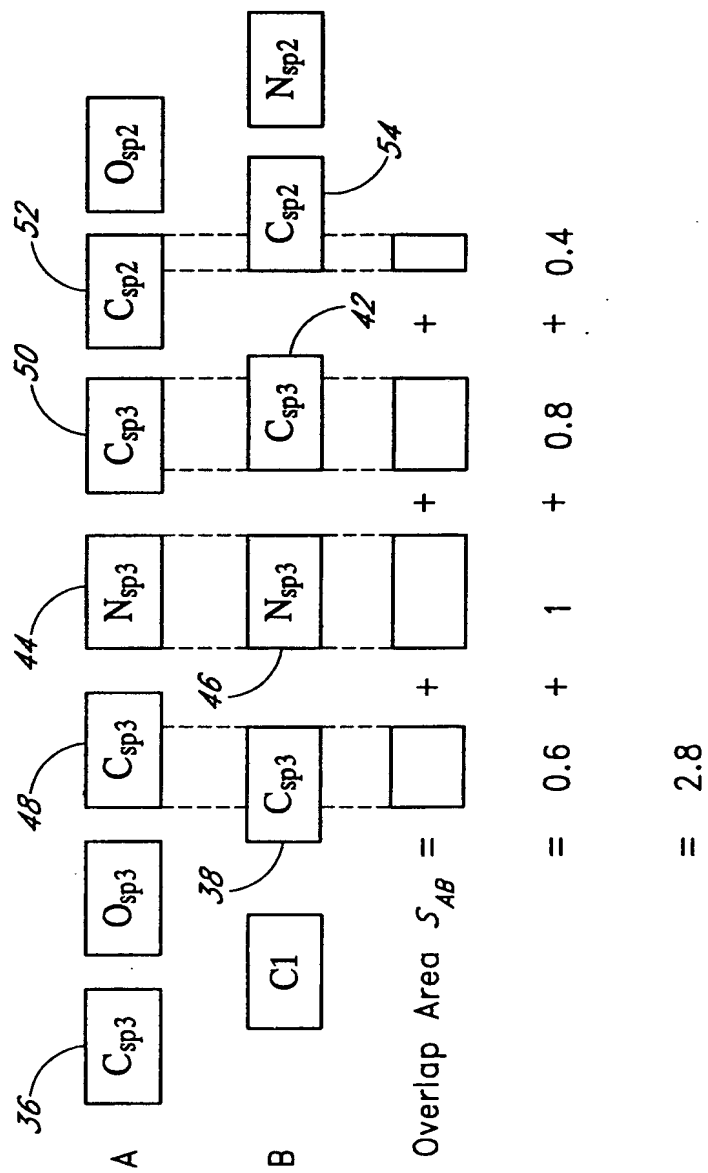


FIG. 3B

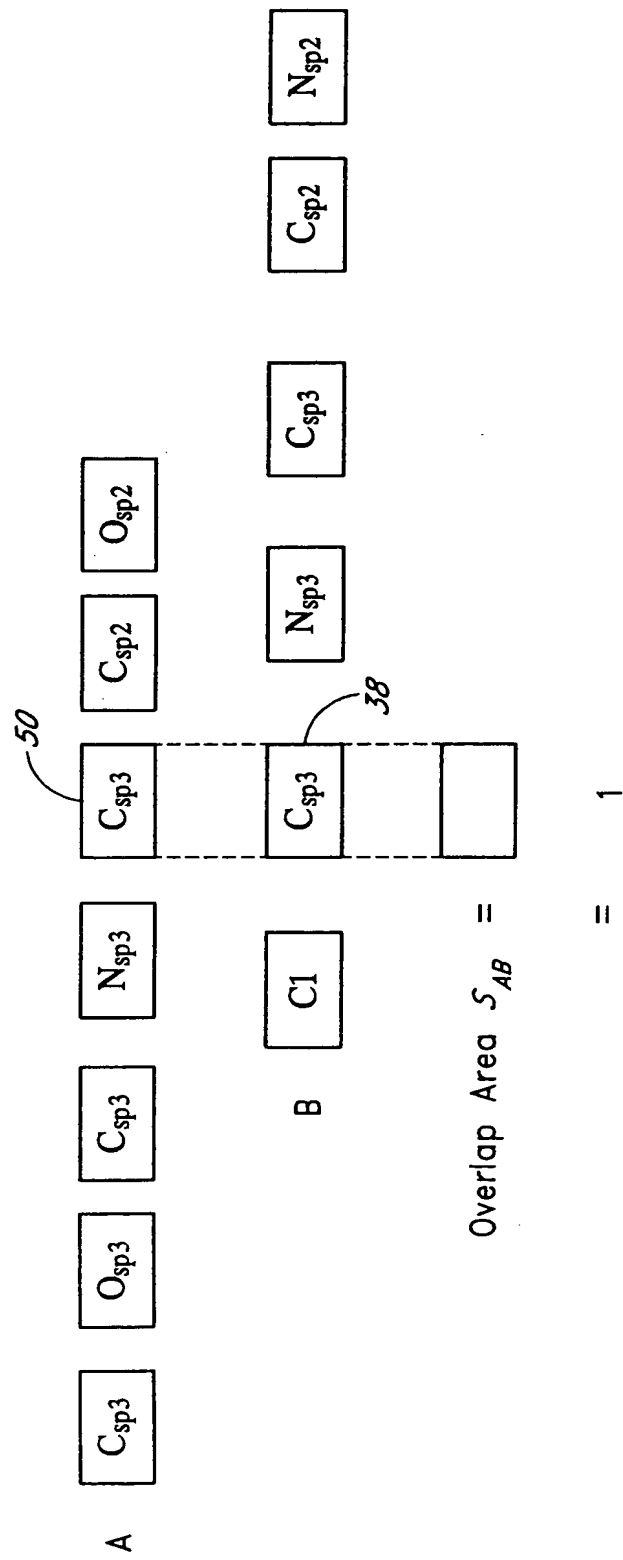


FIG. 3C

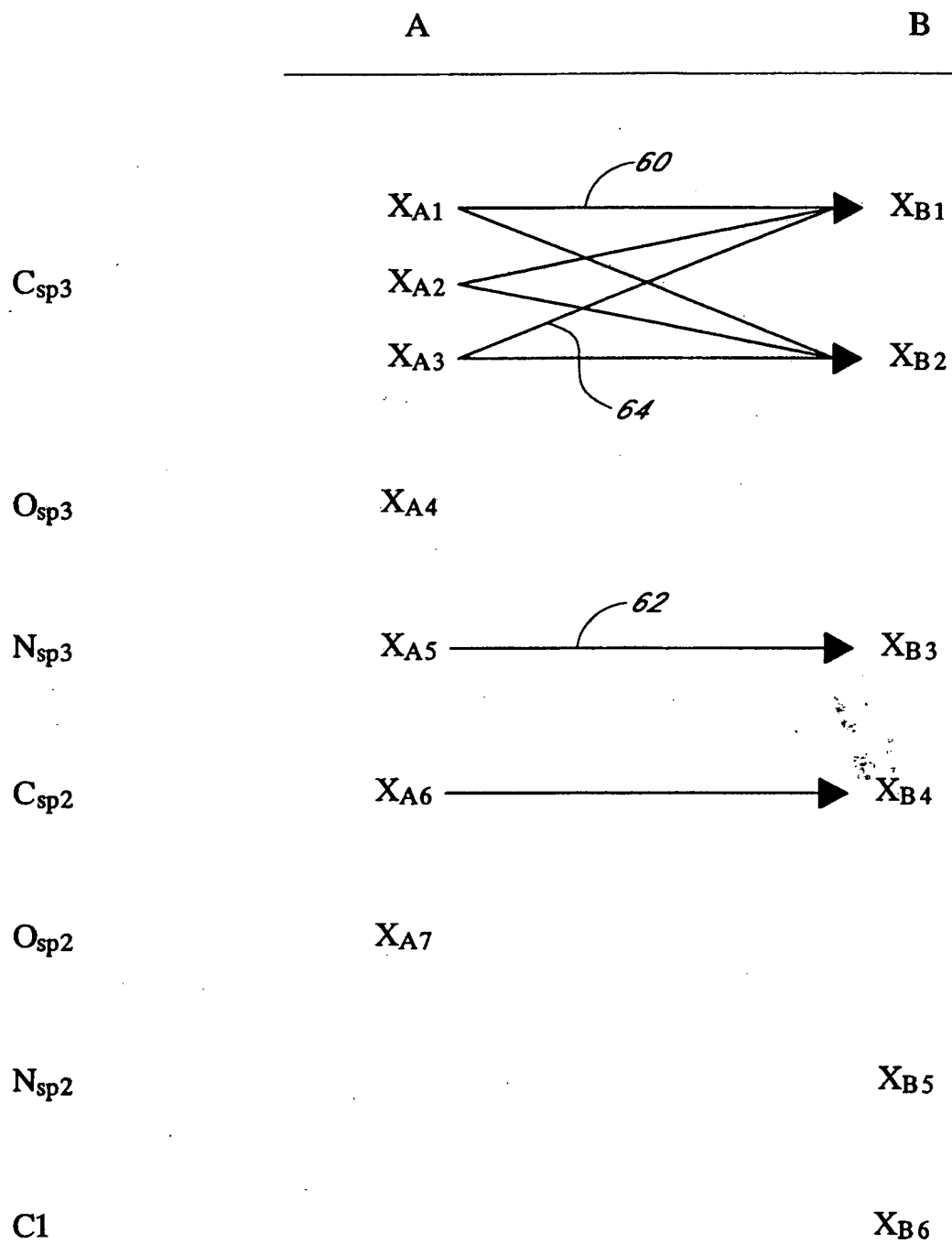


FIG. 4

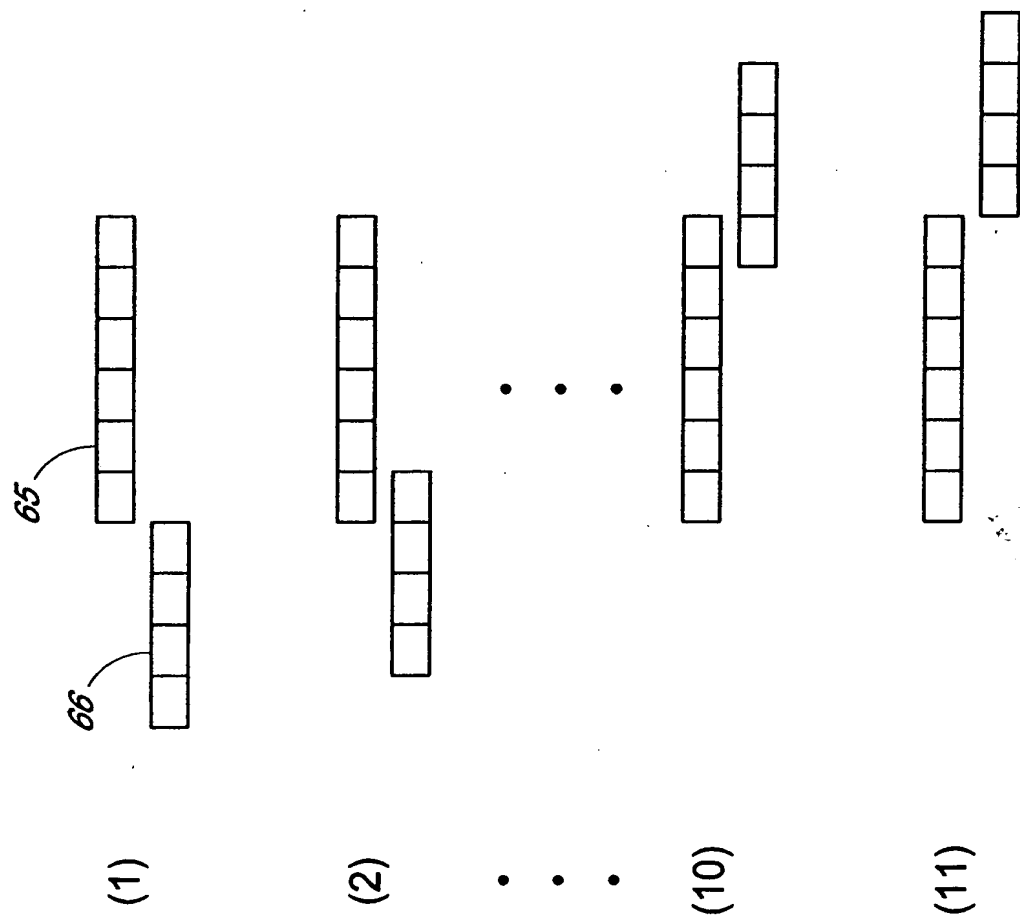


FIG. 5

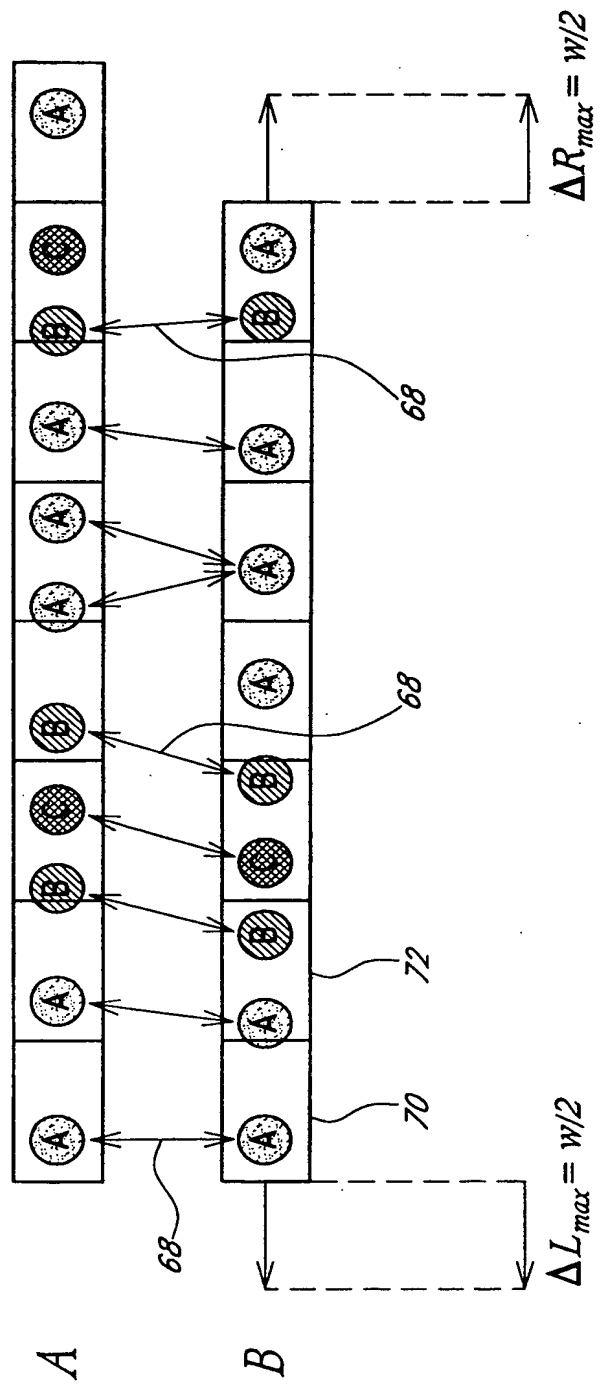


FIG. 6

FIG. 7A A

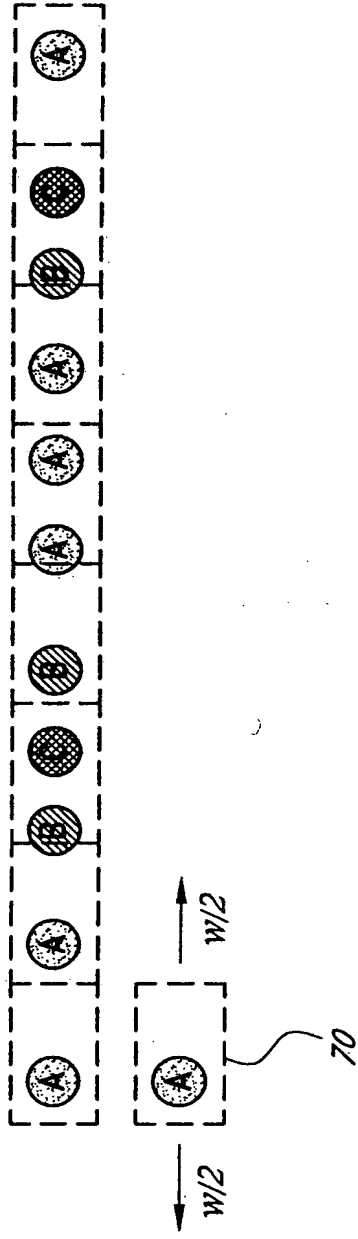


FIG. 7B A

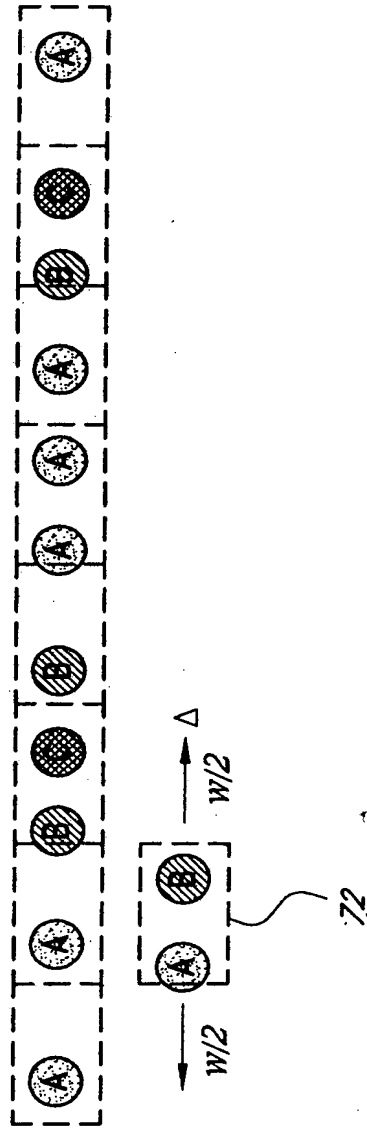
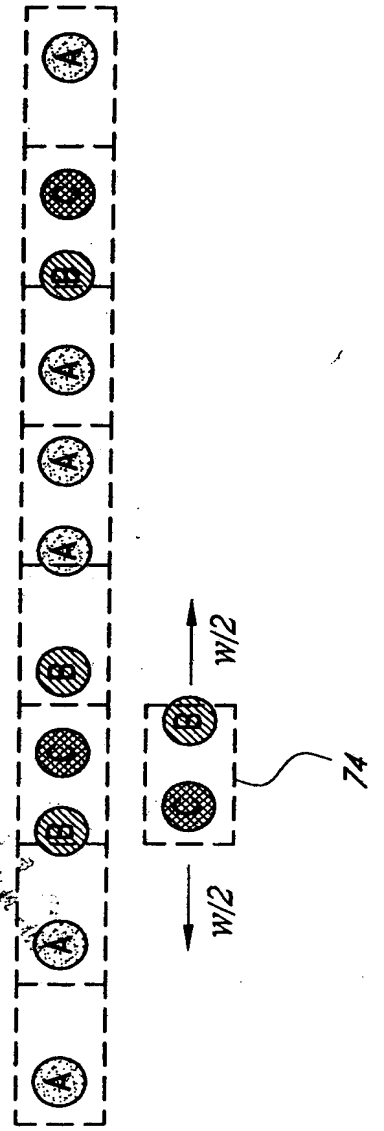


FIG. 7C A



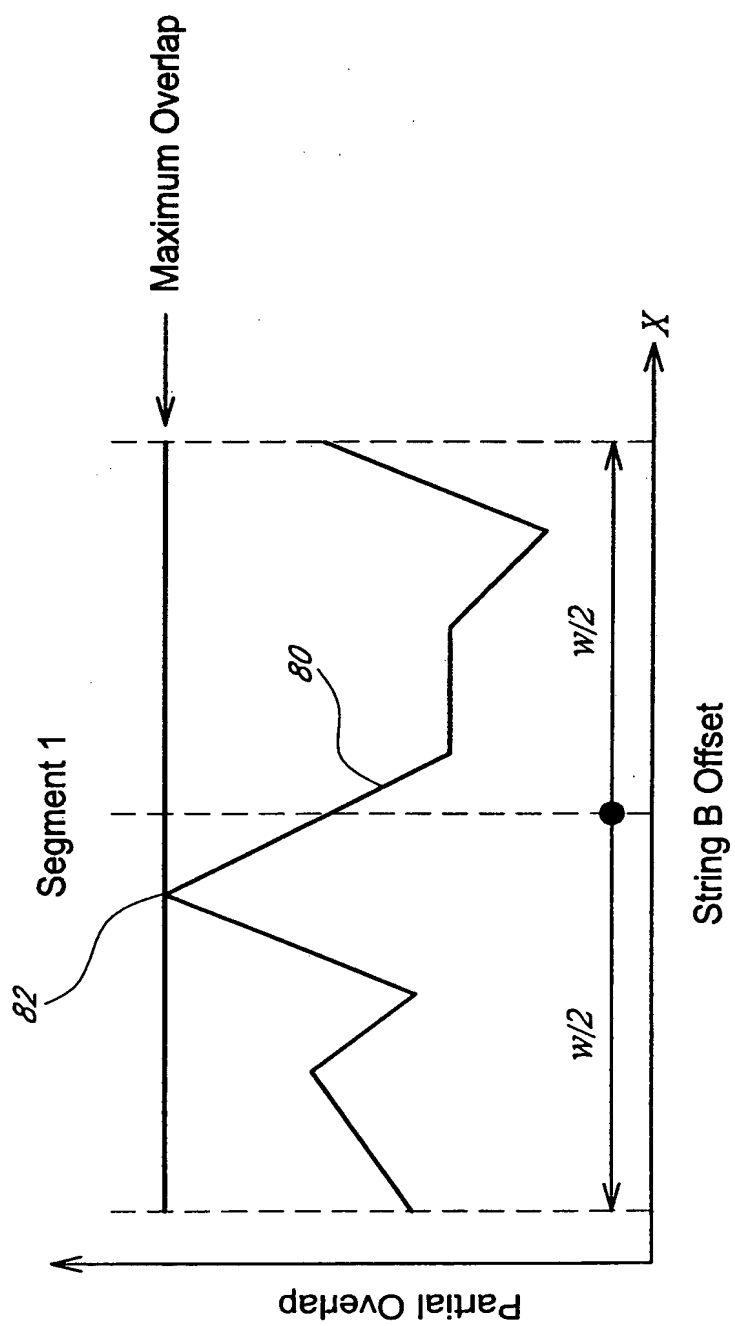


FIG. 8A

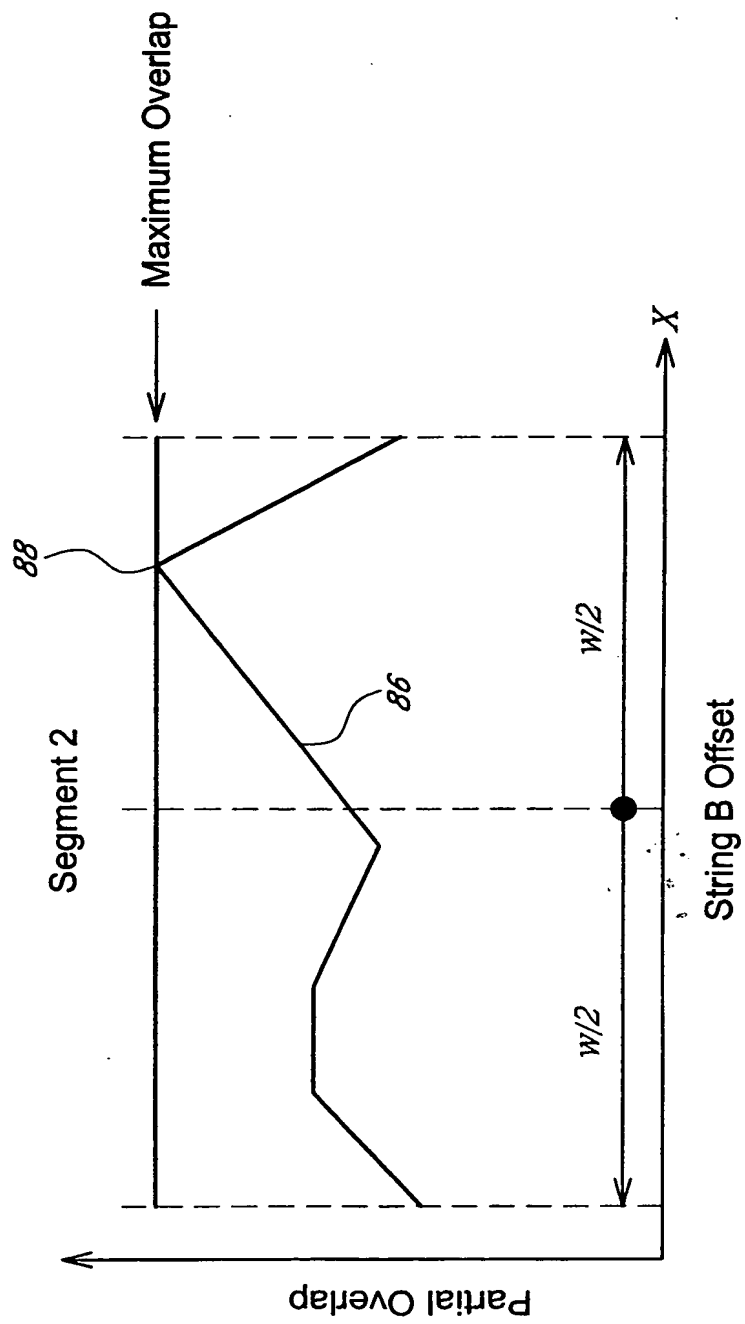


FIG. 8B

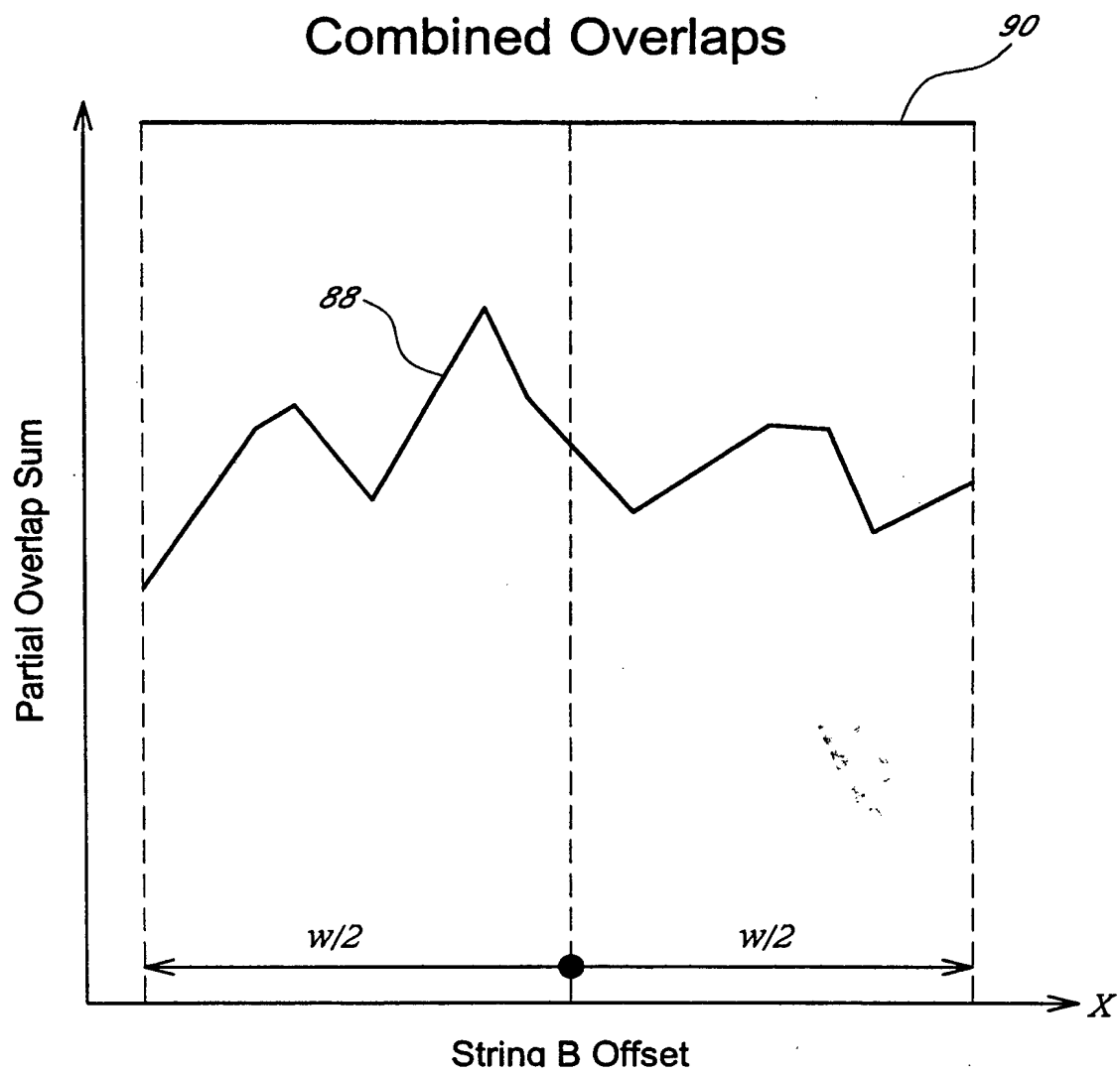
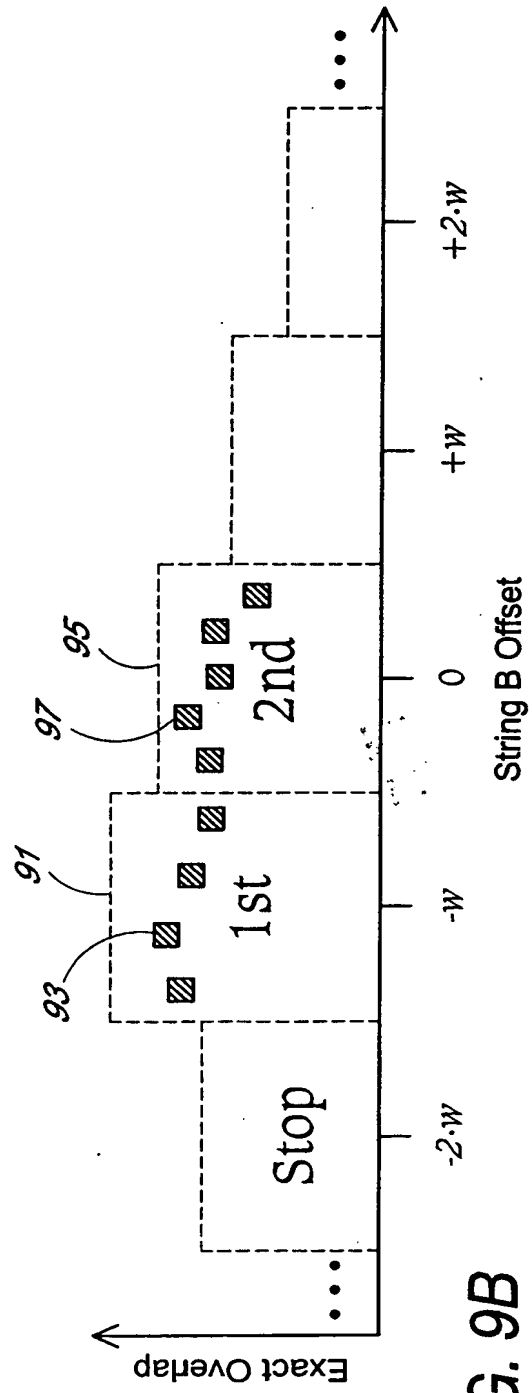
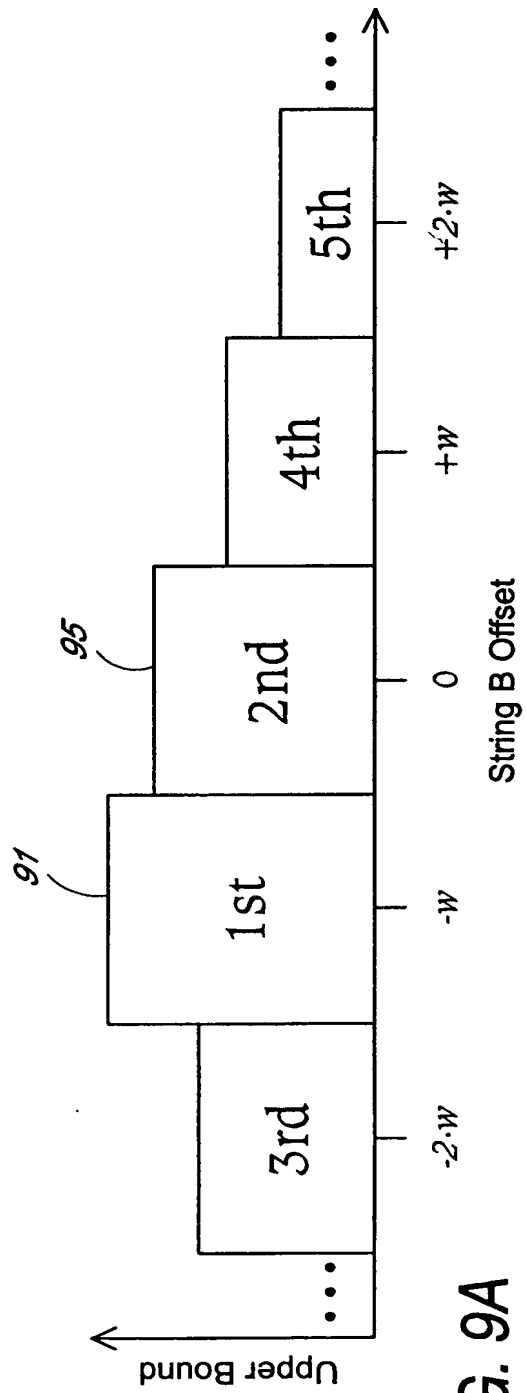


FIG. 8C



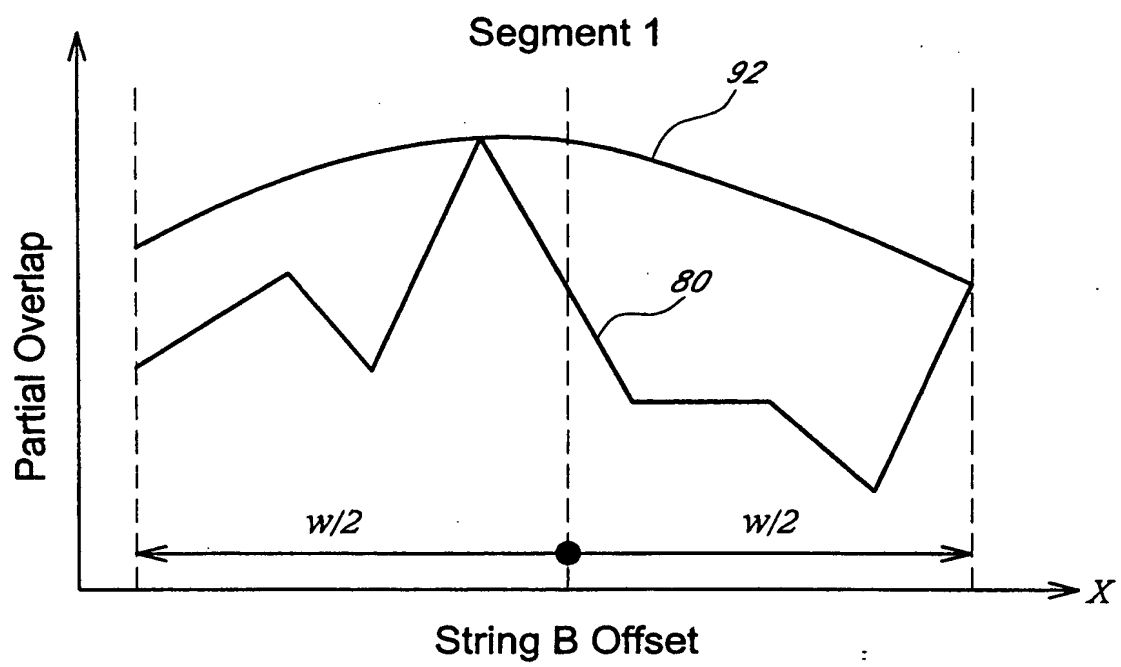


FIG. 10A

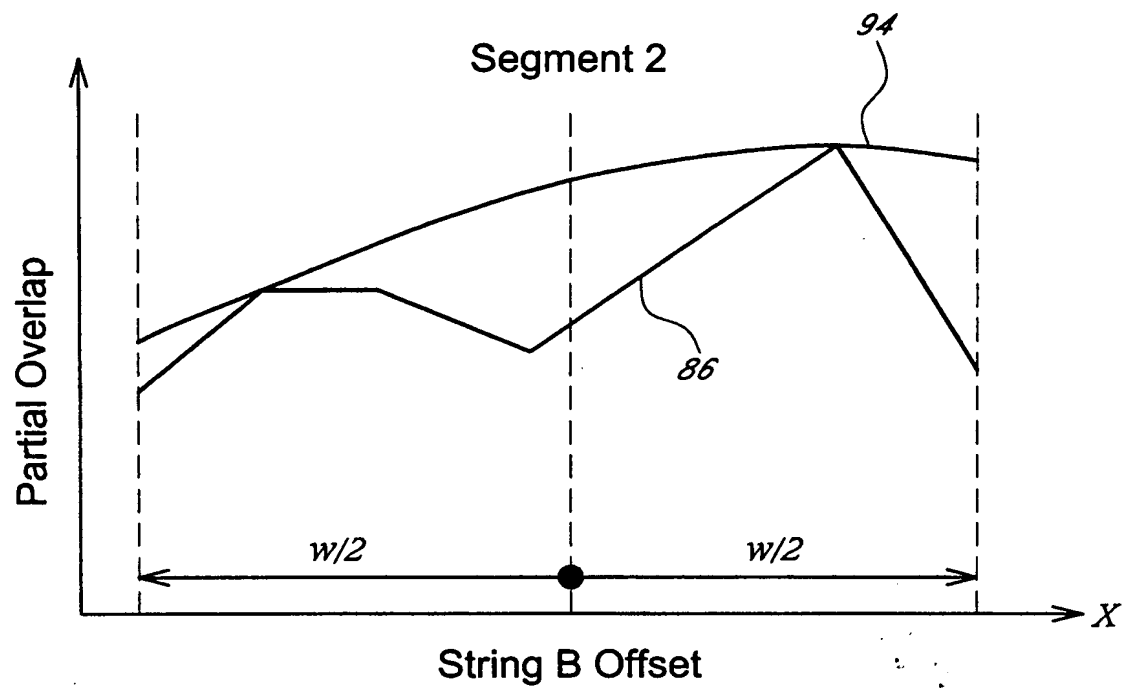


FIG. 10B

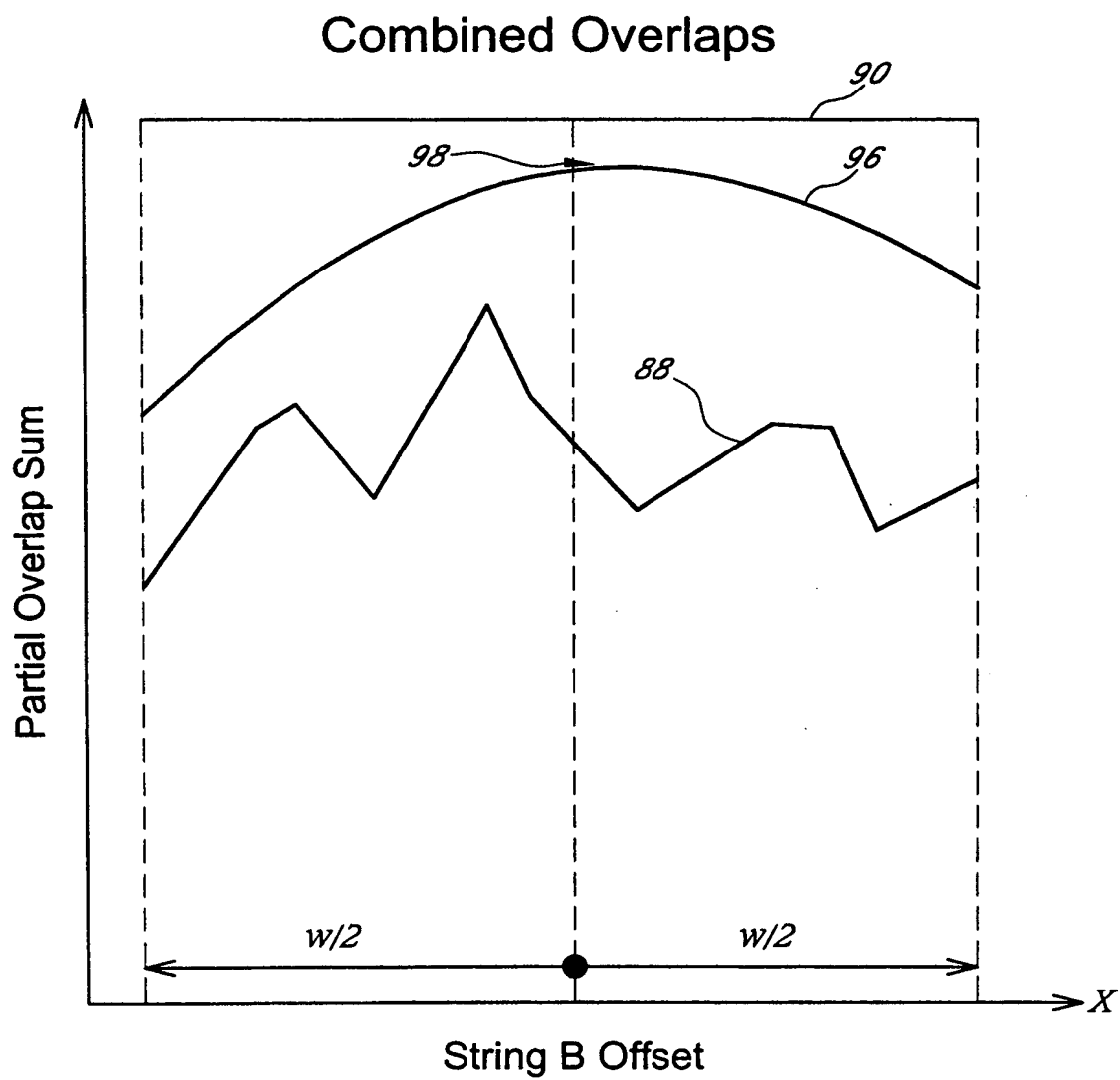
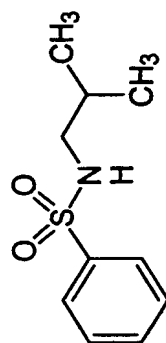
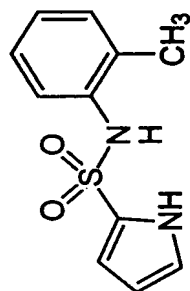


FIG. 10C



Compound A

2D→1D



Compound B1

3D→1D

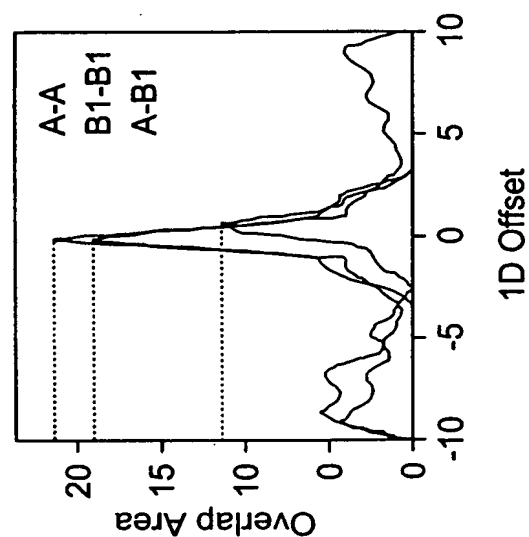
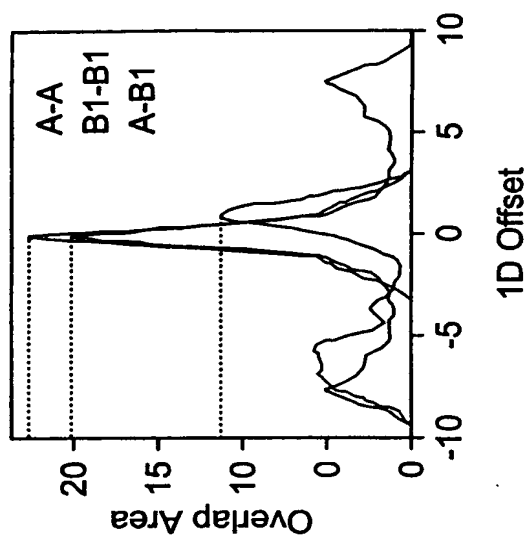
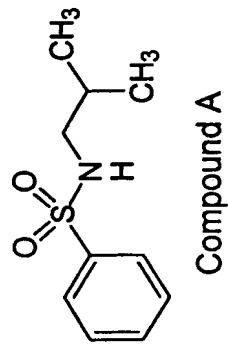


FIG. 11

3D→1D



2D→1D

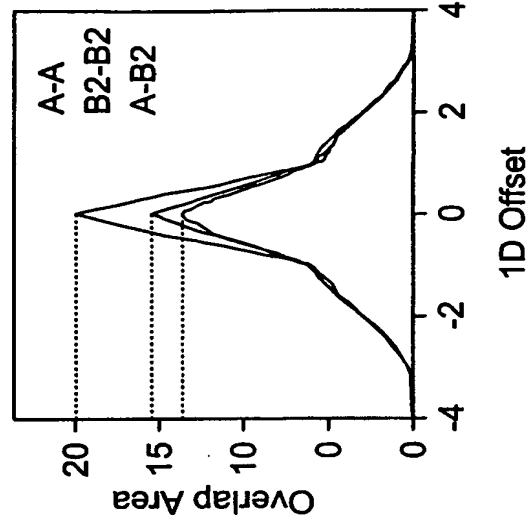
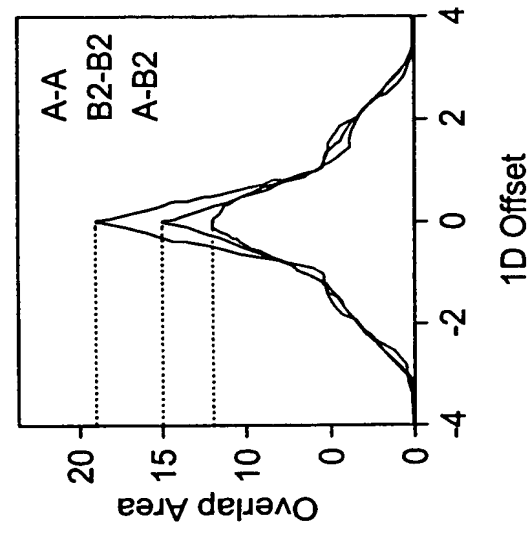
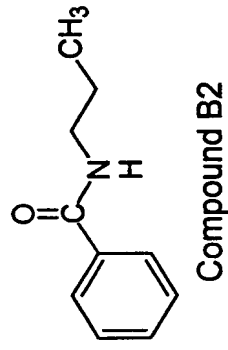


FIG. 12

Bin-Based Overlap

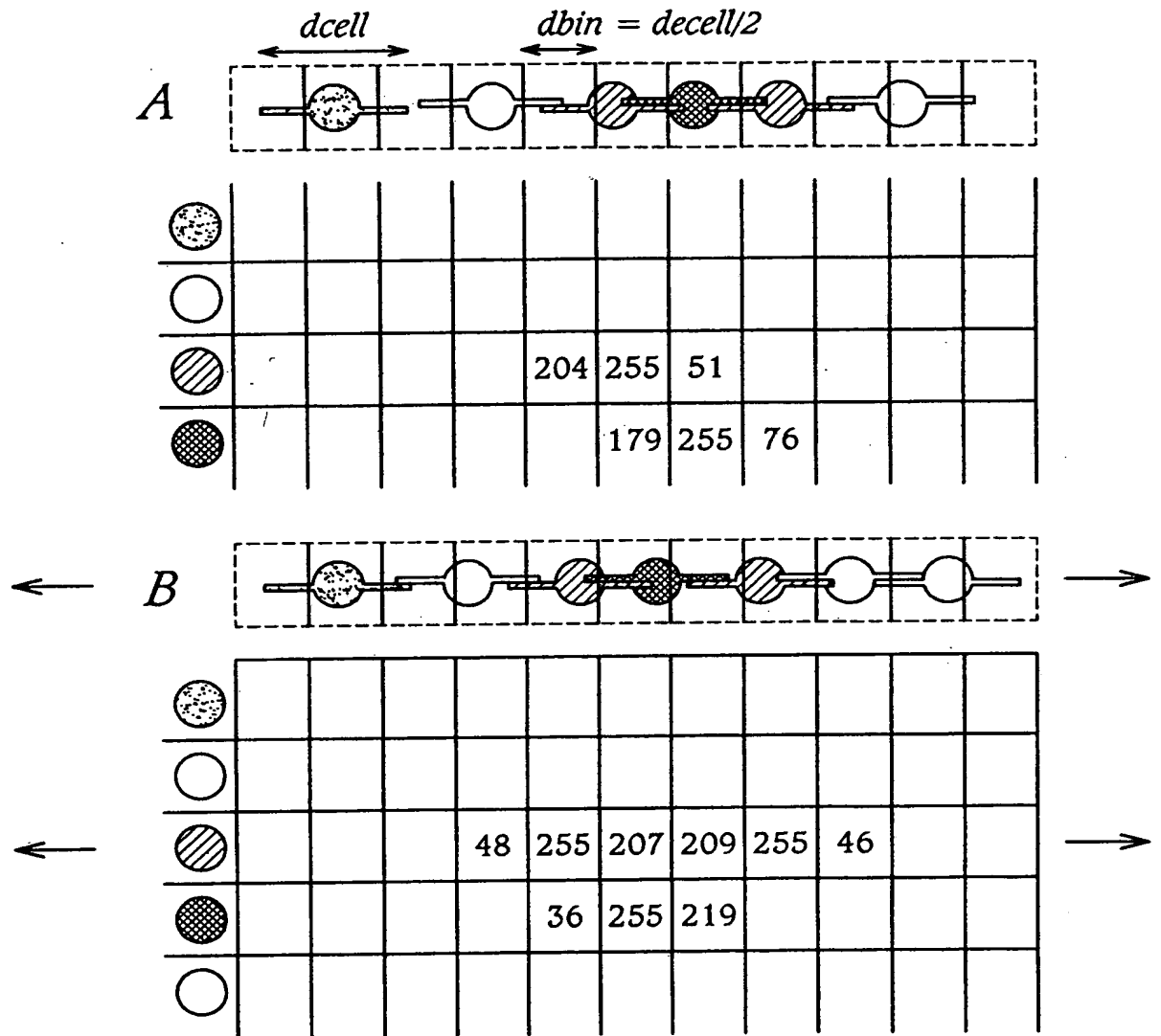


FIG. 13

Speeding Up Bin-Based Overlap Calculations

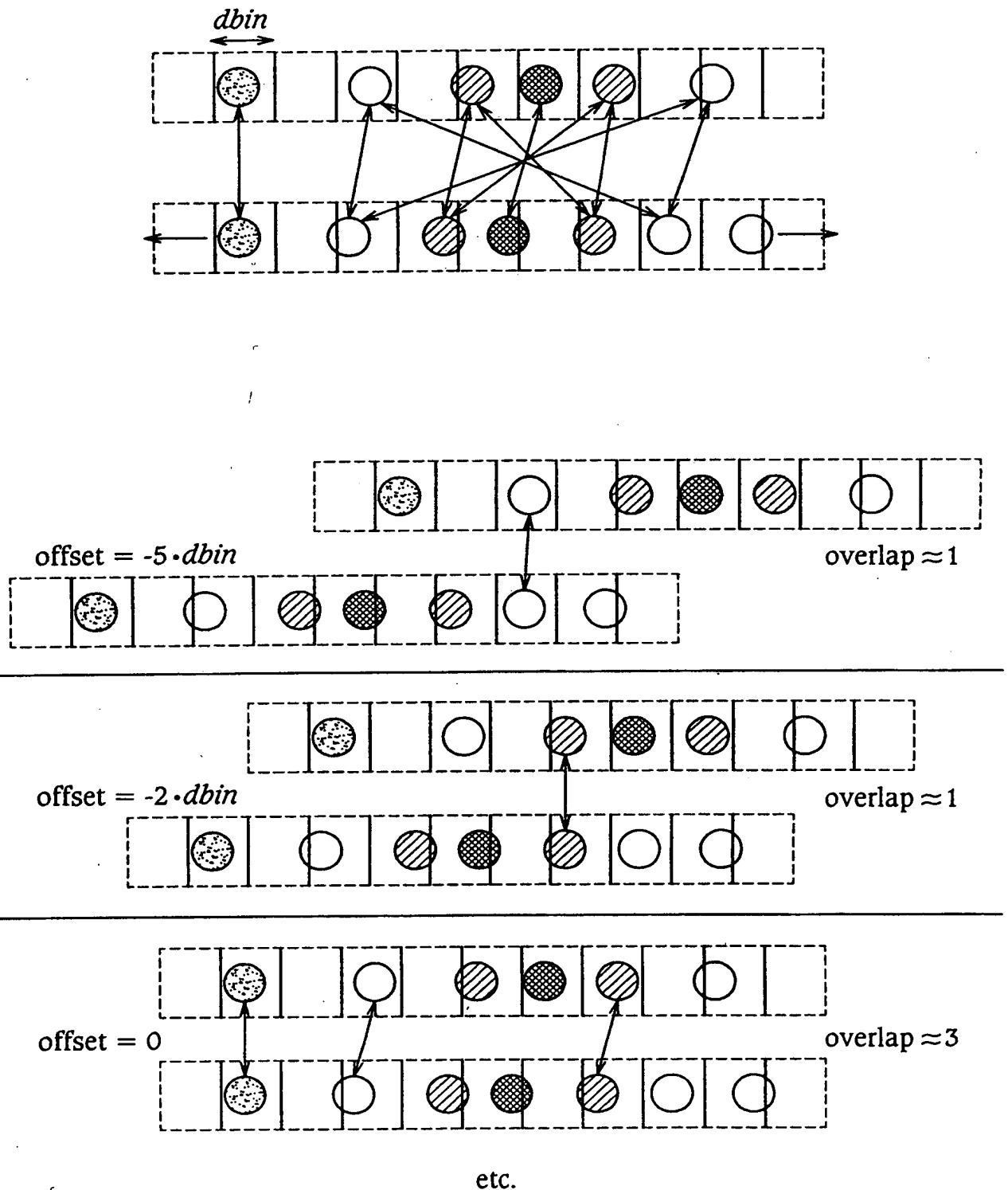


FIG. 14

Approximate Bin-Based Overlaps \rightarrow Upper Bounds

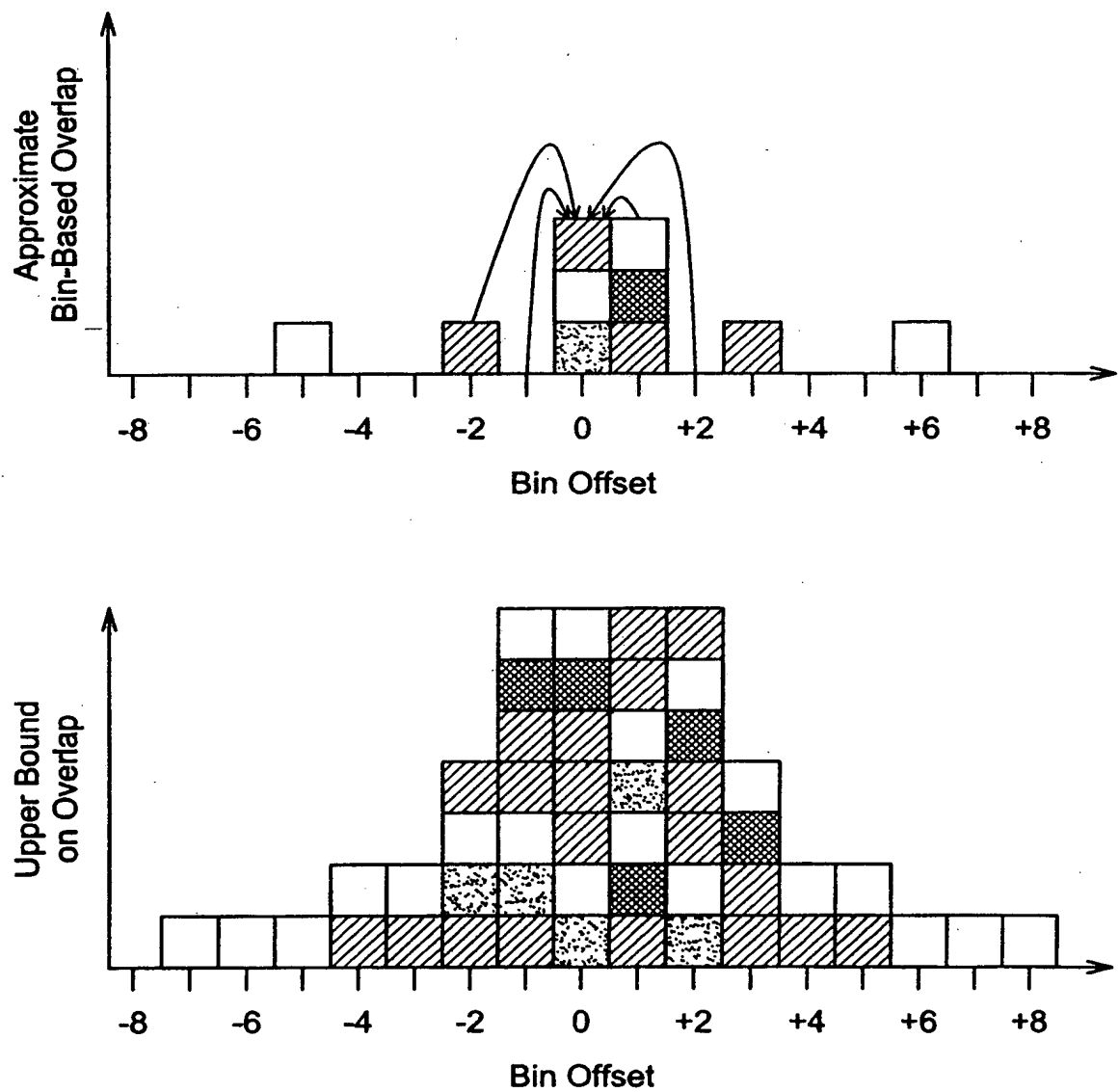


FIG. 15